$%^STN;HighlightOn=;HighlightOff=;

Connecting via Winsock to STN

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * *   Welcome to STN International   * * * * * * * * * * *

```
NEWS  1              Web Page URLs for STN Seminar Schedule - N. America
NEWS  2              "Ask CAS" for self-help around the clock
NEWS  3   OCT 23    The Derwent World Patents Index suite of databases on STN
                    has been enhanced and reloaded
NEWS  4   OCT 30    CHEMLIST enhanced with new search and display field
NEWS  5   NOV 03    JAPIO enhanced with IPC 8 features and functionality
NEWS  6   NOV 10    CA/CAplus F-Term thesaurus enhanced
NEWS  7   NOV·10    STN Express with Discover! free maintenance release Version
                    8.01c now available
NEWS  8   NOV 20    CAS Registry Number crossover limit increased to 300,000 in
                    additional databases
NEWS  9   NOV 20    CA/CAplus to MARPAT accession number crossover limit increased
                    to 50,000
NEWS 10   DEC 01    CAS REGISTRY updated with new ambiguity codes
NEWS 11   DEC 11    CAS REGISTRY chemical nomenclature enhanced
NEWS 12   DEC 14    WPIDS/WPINDEX/WPIX manual codes updated
NEWS 13   DEC 14    GBFULL and FRFULL enhanced with IPC 8 features and
                    functionality
NEWS 14   DEC 18    CA/CAplus pre-1967 chemical substance index entries enhanced
                    with preparation role
NEWS 15   DEC 18    CA/CAplus patent kind codes updated
NEWS 16   DEC 18    MARPAT to CA/CAplus accession number crossover limit increased
                    to 50,000
NEWS 17   DEC 18    MEDLINE updated in preparation for 2007 reload
NEWS 18   DEC 27    CA/CAplus enhanced with more pre-1907 records
NEWS 19   JAN 08    CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 20   JAN 16    CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 21   JAN 16    IPC version 2007.01 thesaurus available on STN
NEWS 22   JAN 16    WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 23   JAN 22    CA/CAplus updated with revised CAS roles
NEWS 24   JAN 22    CA/CAplus enhanced with patent applications from India

NEWS EXPRESS   NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.


NEWS HOURS     STN Operating Hours Plus Help Desk Availability
NEWS LOGIN     Welcome Banner and News Items
NEWS IPC8      For general information regarding STN implementation of IPC 8
```

NEWS X25   X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
specific topic.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:49:12 ON 26 JAN 2007

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                    ENTRY   SESSION
FULL ESTIMATED COST   0.63   0.63

FILE 'REGISTRY' ENTERED AT 08:50:53 ON 26 JAN 2007
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STRUCTURE FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007 HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

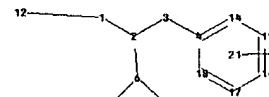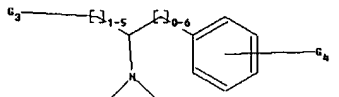TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C.str

```
chain nodes :
1   2   3   5   6   7   12   20
ring nodes :
4   14   15   16   17   18
chain bonds :
1-2   1-12   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-14   4-18   14-15   15-16   16-17   17-18
exact/norm bonds :
1-12   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-14   4-18   14-15   15-16   16-17   17-18


G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

G4:C,O,S,N

Match level :
1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   12:CLASS   14:Atom
15:Atom   16:Atom   17:Atom   18:Atom   20:CLASS   21:Atom



L1        STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1                STR
```
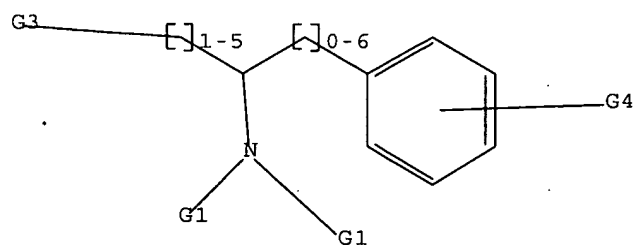
G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy
G4 C,O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 08:51:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   403503 TO ITERATE

   0.5% PROCESSED   2000 ITERATIONS   5 ANSWERS
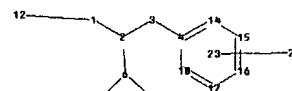INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
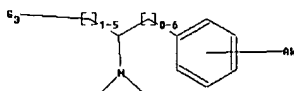SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **INCOMPLETE**
                         BATCH   **INCOMPLETE**
PROJECTED ITERATIONS: 8033707 TO 8106413
PROJECTED ANSWERS: 18270 TO   22080

L2   5 SEA SSS SAM L1

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-1.str .

chain nodes :
1 2 3 5 6 7 12 22
ring nodes :
4 14 15 16 17 18
chain bonds :
1-2 1-12 2-3 2-6 3-4 5-6 6-7
ring bonds :

```
4-14   4-18   14-15   15-16   16-17   17-18
exact/norm bonds :
1-12   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-14   4-18   14-15   15-16  ˙16-17   17-18


G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

G4:C,O,S,N

Match level :
1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   12:CLASS   14:Atom
15:Atom   16:Atom   17:Atom   18:Atom   22:CLASS   23:CLASS



L3          STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                    STR
```
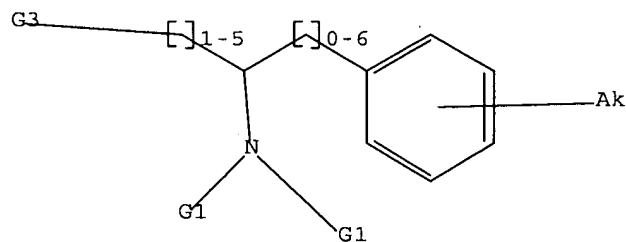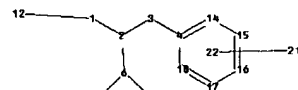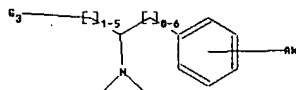


```
G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy
G4 C,O,S,N
```

Structure attributes must be viewed using STN Express query preparation.

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-2.str

```
chain nodes :
1   2   3   5   6   7   12   21
ring nodes :
4   14   15   16   17   18
chain bonds :
1-2   1-12   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-14   4-18   14-15   15-16   16-17   17-18
exact/norm bonds :
1-12   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-14   4-18   14-15   15-16   16-17   17-18


G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

Match level :
1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   12:CLASS   14:Atom
15:Atom   16:Atom   17:Atom   18:Atom   21:CLASS   22:CLASS



L4          STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4                  STR
```
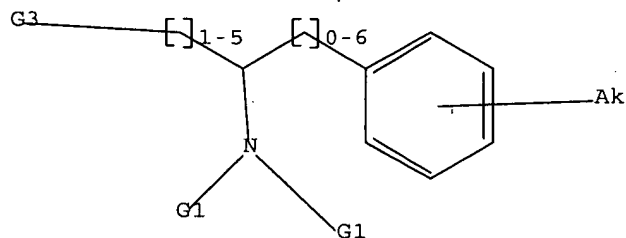
G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 08:56:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   403493 TO ITERATE

   0.5% PROCESSED   2000 ITERATIONS   1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **INCOMPLETE**
                         BATCH   **INCOMPLETE**
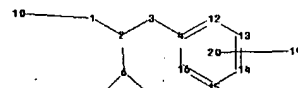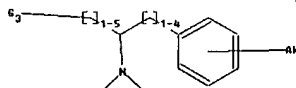PROJECTED ITERATIONS: 8033507 TO   8106213
PROJECTED ANSWERS: 3182 TO   4886

L5   1 SEA SSS SAM L4

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-3.str

chain nodes :
1 2 3 5 6 7 10 19
ring nodes :
4 12 13 14 15 16
chain bonds :
1-2 1-10 2-3 2-6 3-4 5-6 6-7
ring bonds :
4-12 4-16 12-13 13-14 14-15 15-16

exact/norm bonds :
1-10 2-6 5-6 6-7
exact bonds :
1-2 2-3 3-4
normalized bonds :
4-12 4-16 12-13 13-14 14-15 15-16

G1:H,Ak

G3:CO2H,PO3H2,SO3H,P,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 12:Atom
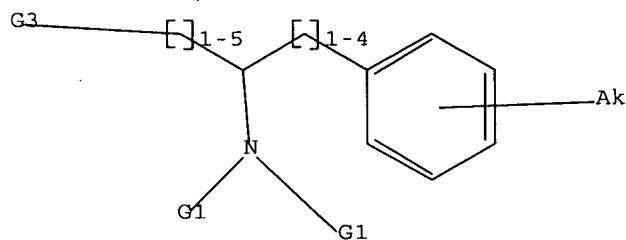13:Atom 14:Atom 15:Atom 16:Atom 19:CLASS 20:CLASS

L6   STRUCTURE UPLOADED

=> d
L6 HAS NO ANSWERS
L6   STR

G1 H,Ak
G2
G3 CO2H,PO3H2,SO3H,P,Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l6
SAMPLE SEARCH INITIATED 08:57:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   149459 TO ITERATE

   1.3% PROCESSED   2000 ITERATIONS   5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **INCOMPLETE**
                         BATCH   **INCOMPLETE**
PROJECTED ITERATIONS: 2966375 TO 3011985
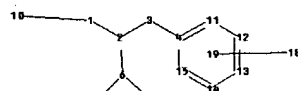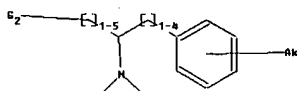PROJECTED ANSWERS: 6313 TO   8631

L7   5 SEA SSS SAM L6

chain nodes :
1   2   3   5   6   7   10   18
ring nodes :
4   11   12   13   14   15
chain bonds :
1-2   1-10   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-11   4-15   11-12   12-13   13-14   14-15
exact/norm bonds :
1-10   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-11   4-15   11-12   12-13   13-14   14-15

G1:H,Ak

G2:CO2H,PO3H2,SO3H,P

Match level :
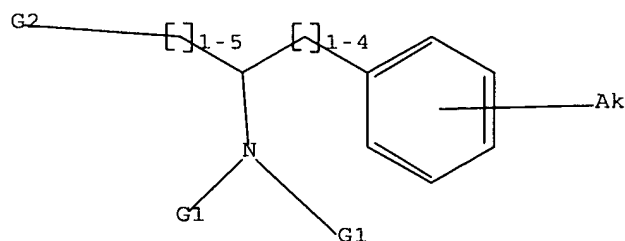1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   10:CLASS   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   18:CLASS   19:CLASS

L8   STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8   STR

G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s 18
SAMPLE SEARCH INITIATED 09:03:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   40869 TO ITERATE

   4.9% PROCESSED   2000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 805306 TO   829454
PROJECTED ANSWERS: 0 TO   0

L9   0 SEA SSS SAM L8

=> s 18 full
FULL SEARCH INITIATED 09:05:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   818627 TO ITERATE

  75.4% PROCESSED   616890 ITERATIONS   252 ANSWERS

  97.7% PROCESSED   799886 ITERATIONS   306 ANSWERS

  98.9% PROCESSED   809895 ITERATIONS   318 ANSWERS

 100.0% PROCESSED   818627 ITERATIONS   318 ANSWERS
SEARCH TIME: 00.00.53

L10   318 SEA SSS FUL L8

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                     ENTRY   SESSION
FULL ESTIMATED COST   183.35   183.98

FILE 'CAPLUS' ENTERED AT 09:06:12 ON 26 JAN 2007
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FILE COVERS 1907 - 26 Jan 2007   VOL 146 ISS 6
FILE LAST UPDATED: 25 Jan 2007   (20070125/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html
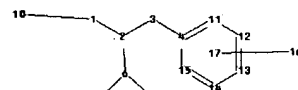
=> s l10
L11   94 L10

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-5.str

chain nodes :
1 2   3   5   6   7   10   16
ring nodes :
4   11   12   13   14   15
chain bonds :
1-2   1-10   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-11   4-15   11-12   12-13   13-14   14-15
exact/norm bonds :
1-10   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-11   4-15   11-12   12-13   13-14   14-15

G1:H,Ak

G2:CO2H,PO3H2,SO3H,P

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:CLASS 6:CLASS 7:CLASS 10:CLASS 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS
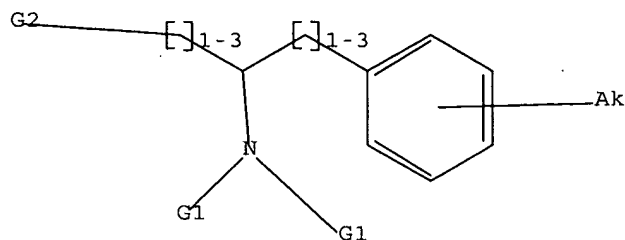

L12   STRUCTURE UPLOADED

=> d
L12 HAS NO ANSWERS
L12   STR

 G1 H,Ak
 G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l12
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:12:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   40869 TO ITERATE

   4.9% PROCESSED   2000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 805306 TO   829454
PROJECTED ANSWERS: 0 TO   0

L13   0 SEA SSS SAM L12

L14   0 L13

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION

FILE 'REGISTRY' ENTERED AT 09:12:46 ON 26 JAN 2007
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STRUCTURE FILE UPDATES: 24 JAN 2007   HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007   HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

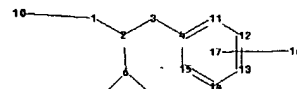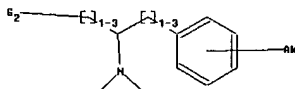TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-5.str

chain nodes :
1   2   3   5   6   7   10   16
ring nodes :
4   11   12   13   14   15
chain bonds :
1-2   1-10   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-11   4-15   11-12   12-13   13-14   14-15
exact/norm bonds :
1-10   2-6   5-6   6-7
exact bonds :
1-2   2-3   3-4
normalized bonds :
4-11   4-15   11-12   12-13   13-14   14-15

G1:H,Ak

G2:CO2H,PO3H2,SO3H,P
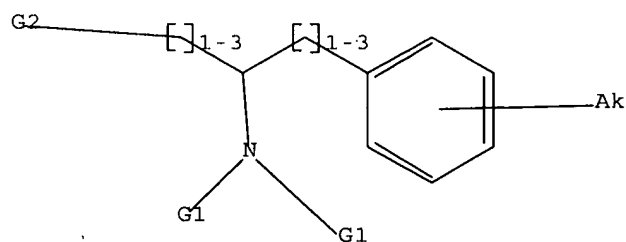
Match level :
1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   10:CLASS   11:Atom
12:Atom   13:Atom   14:Atom   15:Atom   16:CLASS   17:CLASS

L15   STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15   STR

G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l15
SAMPLE SEARCH INITIATED 09:13:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   40869 TO ITERATE

   4.9% PROCESSED   2000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                         BATCH   **COMPLETE**
PROJECTED ITERATIONS: 805306 TO   829454
PROJECTED ANSWERS: 0 TO   0

L16   0 SEA SSS SAM L15

=> s l15
SAMPLE SEARCH INITIATED 09:13:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   40869 TO ITERATE

   4.9% PROCESSED   2000 ITERATIONS   0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**

```
                       BATCH    **COMPLETE**
PROJECTED ITERATIONS:          805306 TO    829454
PROJECTED ANSWERS:                  0 TO         0

L17            0 SEA SSS SAM L15

=> s l15 full
FULL SEARCH INITIATED 09:13:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   818627 TO ITERATE

 87.3% PROCESSED    714743 ITERATIONS                        288 ANSWERS

 98.8% PROCESSED    808958 ITERATIONS                        313 ANSWERS

100.0% PROCESSED    818627 ITERATIONS                        313 ANSWERS
SEARCH TIME: 00.00.39

L18          313 SEA SSS FUL L15

=> file caplus
COST IN U.S. DOLLARS                         SINCE FILE       TOTAL
                                               ENTRY         SESSION
FULL ESTIMATED COST                            173.00         363.07

FILE 'CAPLUS' ENTERED AT 09:14:43 ON 26 JAN 2007
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FILE COVERS 1907 - 26 Jan 2007  VOL 146 ISS 6
FILE LAST UPDATED: 25 Jan 2007   (20070125/ED)

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They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l18
L19          94 L18

=> file reg
COST IN U.S. DOLLARS                         SINCE FILE       TOTAL
                                               ENTRY         SESSION
FULL ESTIMATED COST                              1.41         364.48

FILE 'REGISTRY' ENTERED AT 09:16:26 ON 26 JAN 2007
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STRUCTURE FILE UPDATES: 24 JAN 2007   HIGHEST RN 918400-64-3
DICTIONARY FILE UPDATES: 24 JAN 2007   HIGHEST RN 918400-64-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

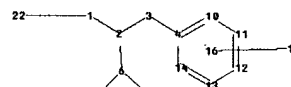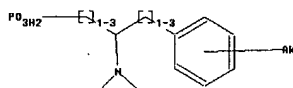TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10505257\10505257C-6.str

chain nodes :
1   2   3   5   6   7   15   22
ring nodes :
4   10   11   12   13   14
chain bonds :
1-2   1-22   2-3   2-6   3-4   5-6   6-7
ring bonds :
4-10   4-14   10-11   11-12   12-13   13-14
exact/norm bonds :
2-6   5-6   6-7
exact bonds :
1-2   1-22   2-3   3-4
normalized bonds :
4-10   4-14   10-11   11-12   12-13   13-14

G1:H,Ak

G2:CO2H,PO3H2,SO3H,P

Match level :
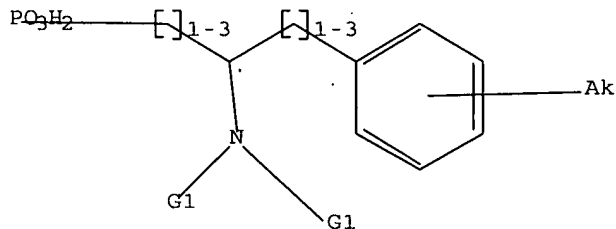1:CLASS   2:CLASS   3:CLASS   4:Atom   5:CLASS   6:CLASS   7:CLASS   10:Atom   11:Atom

12:Atom
13:Atom   14:Atom   15:CLASS   16:CLASS   22:CLASS

L20   STRUCTURE UPLOADED

=> d
L20 HAS NO ANSWERS
L20   STR

G1 H,Ak
G2 CO2H,PO3H2,SO3H,P

Structure attributes must be viewed using STN Express query preparation.

=> s l20
SAMPLE SEARCH INITIATED 09:16:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   72 TO ITERATE

100.0% PROCESSED   72 ITERATIONS   2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE   **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 931 TO   1949
PROJECTED ANSWERS: 2 TO   124

L21   2 SEA SSS SAM L20

=> s l20 full
FULL SEARCH INITIATED 09:17:09 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1470 TO ITERATE

100.0% PROCESSED   1470 ITERATIONS   37 ANSWERS
SEARCH TIME: 00.00.01

L22   37 SEA SSS FUL L20

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION
FULL ESTIMATED COST   172.10   536.58

FILE 'CAPLUS' ENTERED AT 09:17:16 ON 26 JAN 2007

=> s 122
L23   8 L22

=> d ibib abs hitstr tot

L23   ANSWER 1 OF 8   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:465499   CAPLUS   Full-text
DOCUMENT NUMBER: 141:133550
TITLE: The discovery of 3-(N-alkyl)aminopropylphosphonic
                           acids as potent S1P receptor agonists
AUTHOR(S):   Hale, Jeffrey J.; Doherty, George; Toth, Leslie; Li,
                           Zhen; Mills, Sander G.; Hajdu, Richard; Keohane, Carol
                           Ann; Rosenbach, Mark; Milligan, James; Shei, Gan-Ju;
                           Chrebet, Gary; Bergstrom, James; Card, Deborah; Rosen,
                           Hugh; Mandala, Suzanne
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research
                           Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),
                           14(13), 3495-3499
                           CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S):   CASREACT 141:133550
AB   3-(N-Alkyl)aminopropylphosphonic acids are potent agonists of four of the five
      known sphingosine-1-phosphate (S1P) receptor subtypes and are useful in
      immunosuppressive therapy.
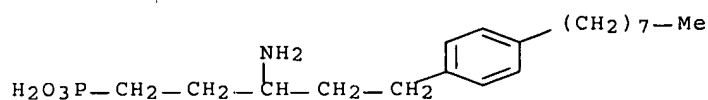IT   596819-84-0 597340-18-6
      RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
      (Biological study); USES (Uses)
          (prepn., immunomodulatory effect and structure-activity relationship
          studies of 3-(N-alkyl)aminopropylphosphonic acids as potent S1P
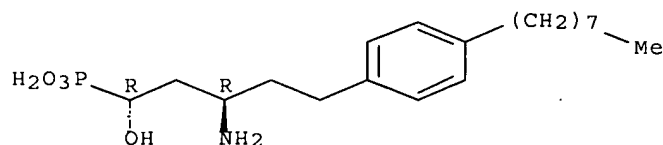   receptor agonists)
RN   596819-84-0 CAPLUS
CN   Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)

$$H_2O_3P-CH_2-CH_2-\underset{\underset{NH_2}{|}}{CH}-CH_2-CH_2-\text{[benzene ring]}-(CH_2)_7-Me$$

Absolute stereochemistry.

$$H_2O_3P-\underset{\underset{OH}{|}}{\overset{R}{C}}-CH_2-\underset{\underset{NH_2}{|}}{\overset{R}{C}}-CH_2-CH_2-\text{[benzene ring]}-(CH_2)_7-Me$$

REFERENCE COUNT: 9   THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
                                   RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

$$Me-(CH_2)_7-\text{[benzene ring]}-CH_2-CH_2-\underset{\underset{NH_2}{|}}{C}-CH_2-\underset{\underset{OH}{|}}{C}-PO_3H_2 \qquad I$$

AB   Alteration in lymphocyte trafficking and prevention of graft rejection in
      rodents obsd. on exposure to FTY720 or its corresponding phosphate ester can

be induced by the systemic administration of potent sphingosine-1-phosphate receptor agonists exemplified by I. The similar S1P receptor profiles of the FTY720 phosphate ester and I coupled with their comparable potency in vivo supports a connection between S1P receptor agonism and immunosuppressive efficacy.

IT   597340-18-6P 597340-22-2P 597340-27-7P
     597340-33-5P
     RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
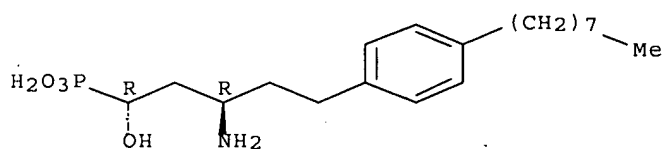   (potent sphingosine-1-phosphate receptor agonists replicate the pharmacol. actions of novel immunosuppressant FTY720 in prevention of graft rejection in relation to alteration in lymphocyte trafficking and pharmacokinetics)

RN   597340-18-6 CAPLUS
CN   Phosphonic acid, [(1R,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
     (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-22-2 CAPLUS
CN   Phosphonic acid, [(1S,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
     (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-27-7 CAPLUS
CN   Phosphonic acid, [(1S,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
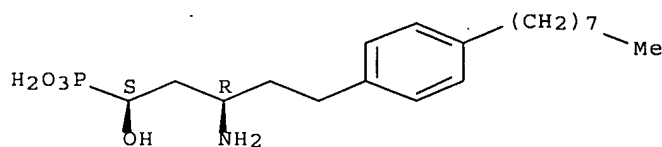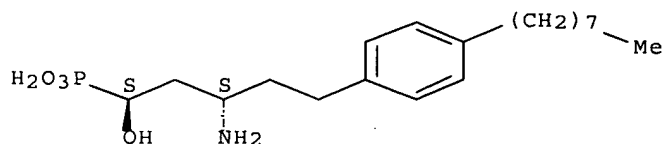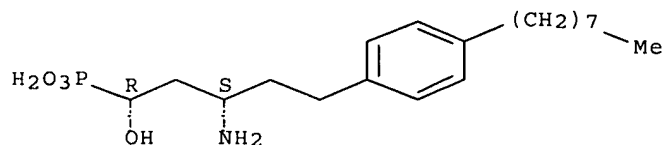   (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-33-5 CAPLUS
CN   Phosphonic acid, [(1R,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
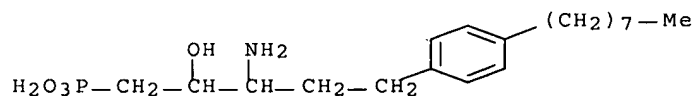   (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

$$H_2O_3P \overset{R}{\underset{OH}{\;}} \overset{S}{\underset{NH_2}{\;}} \text{—(4-octylphenyl)—} (CH_2)_7 \text{—Me}$$

IT   596819-84-0P 596819-85-1P 717888-62-5P
      717888-67-0P
      RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
      (Uses)
          (potent sphingosine-1-phosphate receptor agonists replicate the
          pharmacol. actions of novel immunosuppressant FTY720 in prevention of
          graft rejection in relation to alteration in lymphocyte trafficking and
          pharmacokinetics)
RN   596819-84-0 CAPLUS
CN   Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)
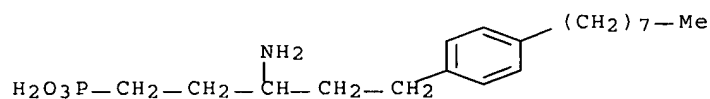
$$H_2O_3P\text{—}CH_2\text{—}CH_2\text{—}\overset{NH_2}{CH}\text{—}CH_2\text{—}CH_2\text{—(4-octylphenyl)—}(CH_2)_7\text{—Me}$$

RN   596819-85-1 CAPLUS
CN   Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI)
      (CA INDEX NAME)

$$H_2O_3P\text{—}CH_2\text{—}\overset{OH}{CH}\text{—}\overset{NH_2}{CH}\text{—}CH_2\text{—}CH_2\text{—(4-octylphenyl)—}(CH_2)_7\text{—Me}$$

RN   717888-62-5 CAPLUS
CN   Phosphonic acid, [3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI)   (CA INDEX
      NAME)

$$H_2O_3P\text{—}CH\text{=}CH\text{—}\overset{NH_2}{CH}\text{—}CH_2\text{—}CH_2\text{—(4-octylphenyl)—}(CH_2)_7\text{—Me}$$
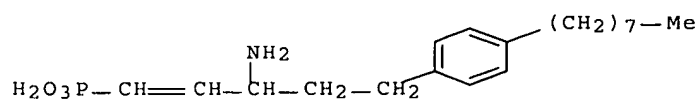
RN   717888-67-0   CAPLUS
CN   Phosphonic acid, [3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI)   (CA
      INDEX NAME)
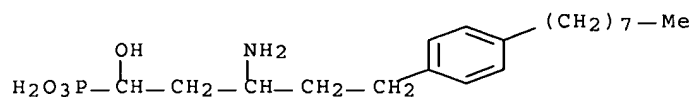
$$H_2O_3P-\overset{\overset{\text{OH}}{|}}{CH}-CH_2-\overset{\overset{\text{NH}_2}{|}}{CH}-CH_2-CH_2-\underset{}{\bigcirc}-(CH_2)_7-Me$$

IT   402615-93-4
      RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
      (Biological study); USES (Uses)
          (potent sphingosine-1-phosphate receptor agonists replicate the
          pharmacol. actions of novel immunosuppressant FTY720 in prevention of
          graft rejection in relation to alteration in lymphocyte trafficking and
          pharmacokinetics)
RN   402615-93-4   CAPLUS
CN   Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]-
      (9CI)   (CA INDEX NAME)

$$H_2O_3P-CH_2-CH_2-\overset{\overset{\text{NH}_2}{|}}{\underset{\underset{\text{HO}-CH_2}{|}}{C}}-CH_2-CH_2-\underset{}{\bigcirc}-(CH_2)_7-Me$$
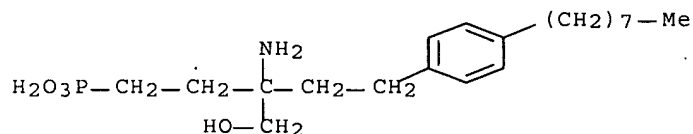
REFERENCE COUNT: 14   THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
                                    RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23   ANSWER 3 OF 8   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:368306   CAPLUS   Full-text
DOCUMENT NUMBER: 141:99302
TITLE: Immune cell regulation and cardiovascular effects of
                            sphingosine 1-phosphate receptor agonists in rodents
                            are mediated via distinct receptor subtypes
AUTHOR(S):   Forrest, M.; Sun, S.-Y.; Hajdu, R.; Bergstrom, J.;
                            Card, D.; Doherty, G.; Hale, J.; Keohane, C.; Meyers,
                            C.; Milligan, J.; Mills, S.; Nomura, N.; Rosen, H.;
                            Rosenbach, M.; Shei, G.-J.; Singer, I. I.; Tian, M.;
                            West, S.; White, V.; Xie, J.; Proia, R. L.; Mandala,
                            S.
CORPORATE SOURCE: Departments of Immunology and Rheumatology,
                            Pharmacology, and Medicinal Chemistry, Merck Research
                            Laboratories, Rahway, NJ, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics
                            (2004), 309(2), 758-768
                            CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental
                            Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB   Sphingosine 1-phosphate (S1P) is a bioactive lysolipid with pleiotropic
     functions mediated through a family of G protein-coupled receptors,
     S1P1,2,3,4,5. Physiol. effects of S1P receptor agonists include regulation of
     cardiovascular function and immunosuppression via redistribution of
     lymphocytes from blood to secondary lymphoid organs. The phosphorylated
     metabolite of the immunosuppressant agent FTY720 (2-amino-2-(2-[4-
     octylphenyl]ethyl)-1,3-propanediol) and other phosphonate analogs with
     differential receptor selectivity were investigated. No significant species
     differences in compd. potency or rank order of activity on receptors cloned
     from human, murine, and rat sources were obsd. All synthetic analogs were
     high-affinity agonists on S1P1, with IC50 values for ligand binding between
     0.3 and 14 nM. The correlation between S1P1 receptor activation and the ED50
     for lymphocyte redn. was highly significant (p < 0.001) and lower for the
     other receptors. In contrast to S1P1-mediated effects on lymphocyte
     recirculation, three lines of evidence link S1P3 receptor activity with acute
     toxicity and cardiovascular regulation: compd. potency on S1P3 correlated with
     toxicity and bradycardia; the shift in potency of phosphorylated-FTY720 for
     inducing lymphopenia vs. bradycardia and hypertension was consistent with
     affinity for S1P1 relative to S1P3; and toxicity, bradycardia, and
     hypertension were absent in S1P3-/- mice. Blood pressure effects of agonists
     in anesthetized rats were complex, whereas hypertension was the predominant
     effect in conscious rats and mice. Immunolocalization of S1P3 in rodent heart
     revealed abundant expression on myocytes and perivascular smooth muscle cells
     consistent with regulation of bradycardia and hypertension, whereas S1P1
     expression was restricted to the vascular endothelium.
IT   719286-66-5 719286-67-6
     RL: PAC (Pharmacological activity); BIOL (Biological study)
         (immune cell regulation and cardiovascular effects of sphingosine
         1-phosphate receptor agonists in rodents are mediated via distinct
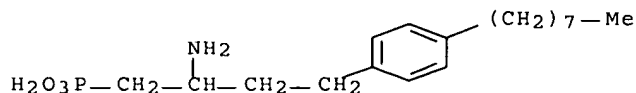   receptor subtypes)
RN   719286-66-5 CAPLUS
CN   Phosphonic acid, [2-amino-2-(hydroxymethyl)-4-(4-octylphenyl)butyl]- (9CI)
     (CA INDEX NAME)
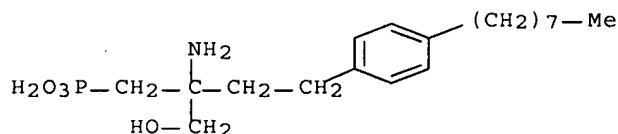
RN   719286-67-6 CAPLUS
CN   Phosphonic acid, [2-amino-4-(4-octylphenyl)butyl]- (9CI)   (CA INDEX NAME)

REFERENCE COUNT: 40   THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:719274 CAPLUS Full-text
DOCUMENT NUMBER: 139:246116
TITLE: Preparation of aminoalkylphosphonates and related
                         compounds as EDG receptor agonists
INVENTOR(S):   Doherty, George A.; Hale, Jeffrey J.
PATENT ASSIGNEE(S):   Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 75 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
        ---------------   ----   --------   ---------------------   --------
        WO 2003074008   A2   20030912   WO 2003-US7262   20030225
        WO 2003074008   A3   20040226
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
                LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
                PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
                UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
                KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
                FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
                BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
        CA 2477449   A1   20030912   CA 2003-2477449   20030225
        AU 2003218056   A1   20030916   AU 2003-218056   20030225
        EP 1482896   A2   20041208   EP 2003-714037   20030225
            R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
        US 2005107345   A1   20050519   US 2003-505268   20030225
        JP 2005531508   T   20051020   JP 2003-572530   20030225
PRIORITY APPLN. INFO.:   US 2002-360605P   P 20020301
                                                  WO 2003-US7262   W 20030225
OTHER SOURCE(S):   MARPAT 139:246116

AB   The present invention encompasses title compds., A-
      X[CR1R2]mCHNH2[CR3R4]pC(R9)3 (m = 1-4; p = 9-20; X = bond, O, NH, S(O)k, k =
      0-2; A = CO2H, PO3H2, PO2H2, SO3H, five membered nitrogen contg. heterocyclyl,
      etc.; two R1 or R3 groups on adjacent carbon may be joined together to form a
      double bond; R2, R3, R4 = H, halo, OH, CO2H, C1-4 alkyl, alkoxy, alkylthio,
      aryl, etc.; R1-R4 = residing on the same carbon optionally joined together to
      form a carbonyl group, etc.; R9 = H, halo, OH, C1-4 alkoxy, alkylthio, C3-7
      cycloalkyl, etc.); as well as the pharmaceutically acceptable salts and
      hydrates thereof. The compds. are useful for treating immune mediated
      diseases and conditions, such as bone marrow, organ and tissue transplant
      rejection. Pharmaceutical compns. and methods of use are included. Thus,
      prepn. of (+/-)-2-amino-4-(4-(octylphenyl))butanol, O-phosphate was described
      in five steps starting from di-Et 2-acetamido-2-(2-(4-
      octylphenyl)ethyl)propanedioate.
IT   596819-82-8P 596819-84-0P 596819-85-1P
      596819-95-3P 596819-96-4P 596819-98-6P
      596819-99-7P 596820-00-7P 596820-06-3P
      596820-07-4P 596820-16-5P 596820-17-6P
      596820-18-7P
      RL: ADV (Adverse effect, including toxicity); BSU (Biological study,
      unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
      (Biological study); PREP (Preparation); USES (Uses)
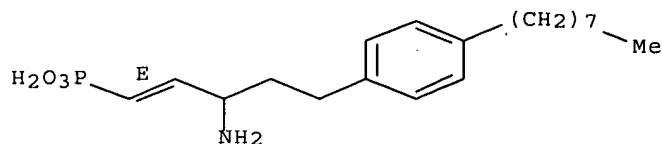   (prepn. of aminoalkylphosphonates and related compds. as EDG receptor

RN   596819-82-8   CAPLUS
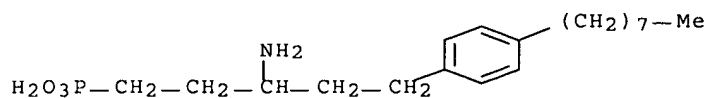CN   Phosphonic acid, [(1E)-3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI)   (CA
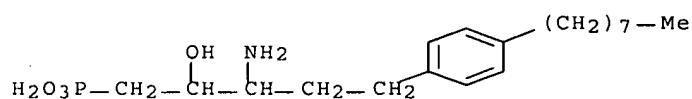   INDEX NAME)

Double bond geometry as shown.

H_2O_3P — CH=CH(E) — CH(NH2) — CH2 — CH2 — C6H4 — (CH2)7 — Me

RN   596819-84-0   CAPLUS
CN   Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)

H_2O_3P—CH2—CH2—CH(NH2)—CH2—CH2—C6H4—(CH2)7—Me

RN   596819-85-1   CAPLUS
CN   Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI)
      (CA INDEX NAME)

H_2O_3P—CH2—CH(OH)—CH(NH2)—CH2—CH2—C6H4—(CH2)7—Me

RN   596819-95-3   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI)
      (CA INDEX NAME)

Absolute stereochemistry.

H_2O_3P—CH(OH)—CH2—CH(R)(NH2)—CH2—CH2—C6H4—(CH2)7—Me

RN   596819-96-4   CAPLUS
CN   Phosphonic acid, [(3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]- (9CI)
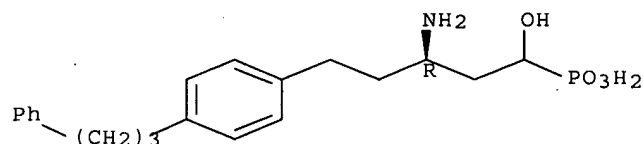   (CA INDEX NAME)

Absolute stereochemistry.

RN   596819-98-6   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(3-
         phenylpropyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
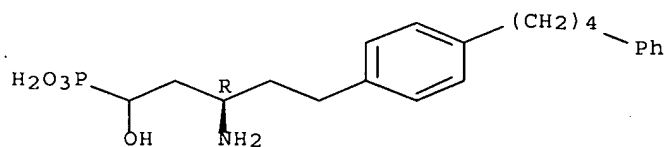
Absolute stereochemistry.

RN   596819-99-7   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(4-
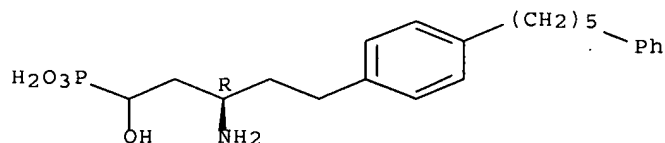   phenylbutyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   596820-00-7   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(5-
         phenylpentyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
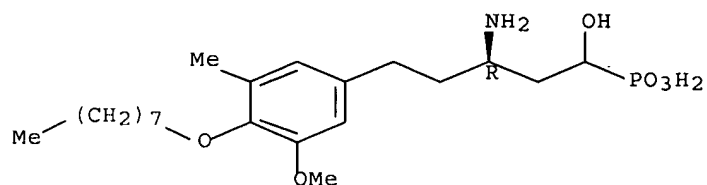
Absolute stereochemistry.

RN   596820-06-3   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[3-methoxy-5-methyl-4-
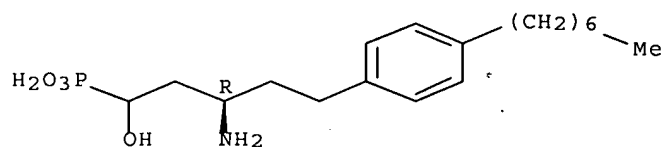   (octyloxy)phenyl]pentyl]- (9CI)   (CA INDEX NAME)

Absolute stereochemistry.
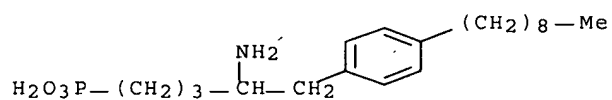

RN   596820-07-4   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-5-(4-heptylphenyl)-1-hydroxypentyl]- (9CI)
       (CA INDEX NAME)
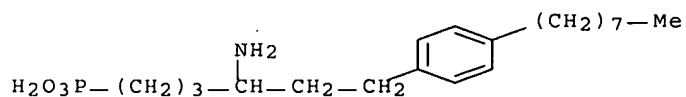
Absolute stereochemistry.

RN   596820-16-5   CAPLUS
CN   Phosphonic acid, [4-amino-5-(4-nonylphenyl)pentyl]- (9CI)   (CA INDEX NAME)
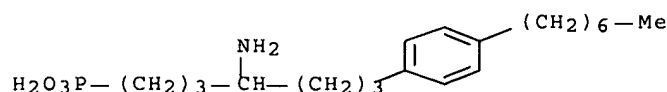

RN   596820-17-6   CAPLUS
CN   Phosphonic acid, [4-amino-6-(4-octylphenyl)hexyl]- (9CI)   (CA INDEX NAME)

RN   596820-18-7   CAPLUS
CN   Phosphonic acid, [4-amino-7-(4-heptylphenyl)heptyl]- (9CI)   (CA INDEX
       NAME)

$$H_2O_3P-(CH_2)_3-\underset{\underset{\displaystyle NH_2}{|}}{CH}-(CH_2)_3-\text{[C}_6\text{H}_4\text{]}-(CH_2)_6-Me$$

L23   ANSWER 5 OF 8   CAPLUS   COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:719253   CAPLUS   Full-text
DOCUMENT NUMBER: 139:245479
TITLE: Preparation of aminoalkylphosphonates and related
                           compounds as EDG receptor agonists
INVENTOR(S):   Budhu, Richard J.; Doherty, George A.; Hale, Jeffrey
                           J.; Lynch, Christopher L.; Mills, Sander G.; Neway,
                           William E., III
PATENT ASSIGNEE(S):   Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 90 pp.
                           CODEN: PIXXD2

Current app.

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO   DATE
        --------------   ----   --------   ------------------   --------
        WO 2003073986   A2   20030912   WO 2003-US5947   20030227
        WO 2003073986   A3   20040527
            W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
                LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
                PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
                UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
                KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
                FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
                BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
        CA 2477423   A1   20030912   CA 2003-2477423   20030227
        AU 2003217764   A1   20030916   AU 2003-217764   20030227
        EP 1482895   A2   20041208   EP 2003-713727   20030227
            R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
        JP 2005531506   T   20051020   JP 2003-572508   20030227
        US 2006089334   A1   20060427   US 2004-505257   20040819
PRIORITY APPLN. INFO.:   US 2002-360663P   P 20020301
                                                WO 2003-US5947   W 20030227
OTHER SOURCE(S):   MARPAT 139:245479
AB   AX(CR1R2)mCH(NH2)(CR3R4)nArBC [A = CO2H, P(O)(OH)2, PH(O)(OH),SO3H, P(O)R5OH,
      5-membered N heterocycle; X = bond, O, NH, S, S, S(O), SO2; R1-R4 = H,
      halogen, OH, CO2H, (un)substituted alkyl, alkoxy, alkylthio, aryl; R1R2, R3R4
      = O; m = 1-4; n = 0-4; R5 = (un)substituted alkyl, aryl; Ar = Ph, naphthyl; C
      = (un)substituted alkyl, alkoxy, acyl, hydroxyalkyl, Ph, heterocyclic, bond;
      when C = bond, B = (un)substituted Ph, alkyl, alkenyl, alkynyl, OH, SH, acyl,
      CONH2, NH2; when C = Ph, heterocyclic, B = (un)substituted alkyl, alkoxy,
      acyl, CO, CH(OH), C6H4, heterocyclic; when C = alkyl, alkoxy, acyl, B =
      (un)substituted C6H4, heterocyclic] were prepd. for use as EDG receptor
      antagonists useful for treating immune mediated diseases and conditions, such
      as bone marrow, organ and tissue transplant rejection (no data). Thus, 4-
   Me(CH2)7C6H4CH2CH2C(NHAc)(CO2Et)2 was hydrolyzed and decarboxylated to 4-

Me(CH2)7C6H4CH2CH2CH(NH2)CO2H which was N-benzyloxycarbonylated, reduced to 4-Me(CH2)7C6H4CH2CH2CH(NHCbz)CH2OH , phosphorylated (MeCH)2NP(OCH2Ph)2, and deblocked to give 4-Me(CH2)7C6H4CH2CH2CH(NH2)CH2OP(O)(OH)2.

IT   596819-82-8P 596819-84-0P 596819-85-1P
    596819-98-6P 596819-99-7P 596820-00-7P
    596820-06-3P 596820-07-4P 597340-18-6P
    597340-22-2P 597340-27-7P 597340-33-5P
    597341-16-7P 597341-24-7P
    RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
      (prepn. of aminoalkylphosphonates and related compds. as EDG receptor agonists)

RN   596819-82-8 CAPLUS
CN   Phosphonic acid, [(1E)-3-amino-5-(4-octylphenyl)-1-pentenyl]- (9CI)   (CA INDEX NAME)

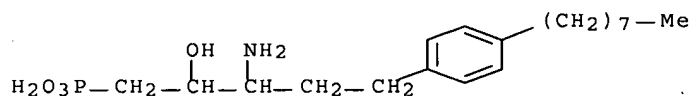Double bond geometry as shown.
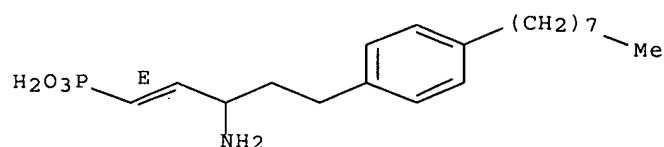
RN   596819-84-0 CAPLUS
CN   Phosphonic acid, [3-amino-5-(4-octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)
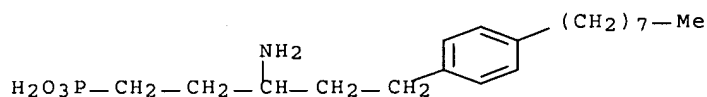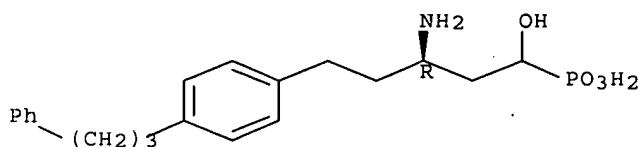

RN   596819-85-1 CAPLUS
CN   Pentitol, 3-amino-1,2,3,5-tetradeoxy-1-(4-octylphenyl)-5-phosphono- (9CI) (CA INDEX NAME)

RN   596819-98-6 CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(3-phenylpropyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
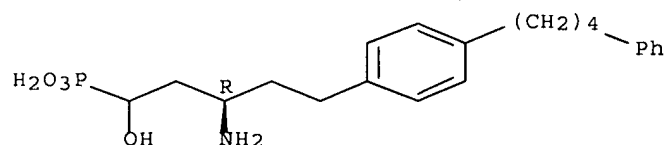
Absolute stereochemistry.

RN   596819-99-7   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(4-
      phenylbutyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
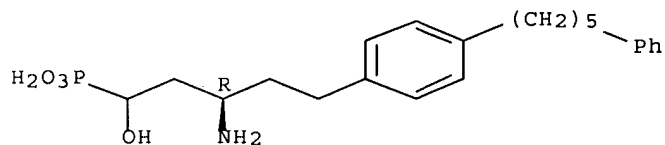
Absolute stereochemistry.

RN   596820-00-7   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[4-(5-
      phenylpentyl)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
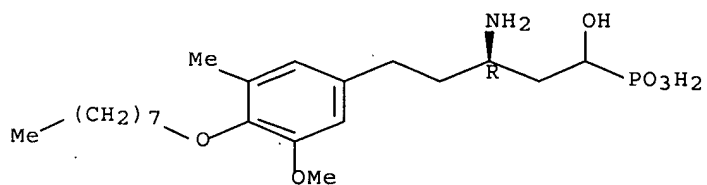
Absolute stereochemistry.

RN   596820-06-3   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-1-hydroxy-5-[3-methoxy-5-methyl-4-
      (octyloxy)phenyl]pentyl]- (9CI)   (CA INDEX NAME)
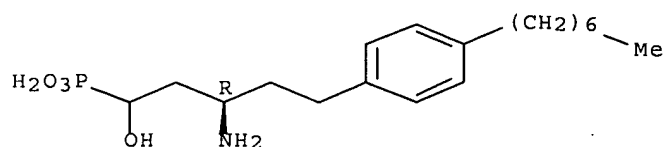
Absolute stereochemistry.

RN   596820-07-4   CAPLUS
CN   Phosphonic acid, [(3R)-3-amino-5-(4-heptylphenyl)-1-hydroxypentyl]- (9CI)
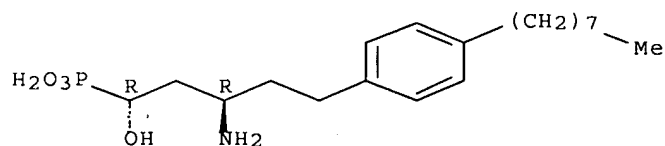   (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-18-6   CAPLUS
CN   Phosphonic acid, [(1R,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
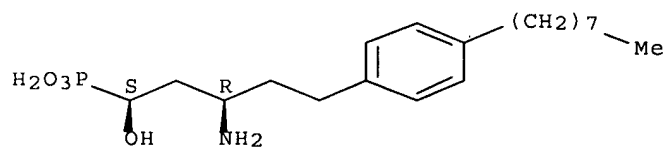   (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-22-2   CAPLUS
CN   Phosphonic acid, [(1S,3R)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
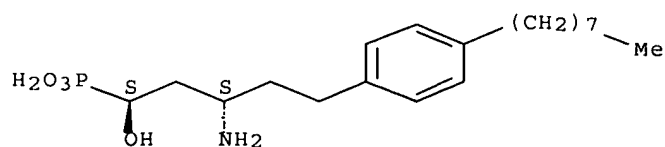   (9CI)   (CA INDEX NAME)

Absolute stereochemistry.

RN   597340-27-7   CAPLUS
CN   Phosphonic acid, [(1S,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
      (9CI)   (CA INDEX NAME)
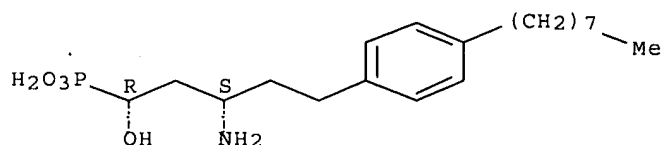
Absolute stereochemistry.
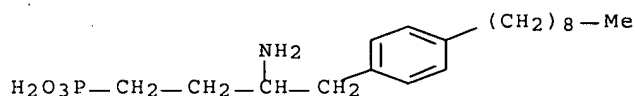

RN   597340-33-5   CAPLUS

CN   Phosphonic acid, [(1R,3S)-3-amino-1-hydroxy-5-(4-octylphenyl)pentyl]-
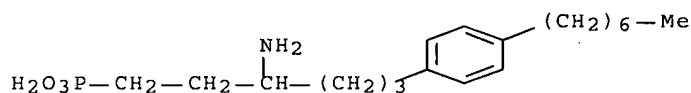   (9CI) (CA INDEX NAME)

Absolute stereochemistry.

H_2O_3P—R—...—S—...—phenyl—$(CH_2)_7$—Me
     OH NH_2

RN   597341-16-7 CAPLUS
CN   Phosphonic acid, [3-amino-4-(4-nonylphenyl)butyl]- (9CI)   (CA INDEX NAME)

$(CH_2)_8$—Me

H_2O_3P—CH_2—CH_2—$\overset{NH_2}{CH}$—CH_2—phenyl—$(CH_2)_8$—Me

RN   597341-24-7 CAPLUS
CN   Phosphonic acid, [3-amino-6-(4-heptylphenyl)hexyl]- (9CI)   (CA INDEX NAME)

$(CH_2)_6$—Me

H_2O_3P—CH_2—CH_2—$\overset{NH_2}{CH}$—$(CH_2)_3$—phenyl—$(CH_2)_6$—Me

L23 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:301209 CAPLUS Full-text
DOCUMENT NUMBER: 137:241872
TITLE: Alteration of lymphocyte trafficking by
                         sphingosine-1-phosphate receptor agonists
AUTHOR(S):   Mandala, Suzanne; Hajdu, Richard; Bergstrom, James;
                         Quackenbush, Elizabeth; Xie, Jenny; Milligan, James;
                         Thornton, Rosemary; Shei, Gan-Ju; Card, Deborah;
                         Keohane, Carolann; Rosenbach, Mark; Hale, Jeffrey;
                         Lynch, Christopher L.; Rupprecht, Kathleen; Parsons,
                         William; Rosen, Hugh
CORPORATE SOURCE: Departments of Immunology and Rheumatology, Merck Res.
                         Laboratories, Rahway, NJ, 07065, USA
SOURCE: Science (Washington, DC, United States) (2002),
                         296(5566), 346-349
                         CODEN: SCIEAS; ISSN: 0036-8075
PUBLISHER: American Association for the Advancement of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
AB   Blood lymphocyte nos., essential for the development of efficient immune
      responses, are maintained by recirculation through secondary Lymphoid organs.
      We show that lymphocyte trafficking is altered by the lysophospholipid
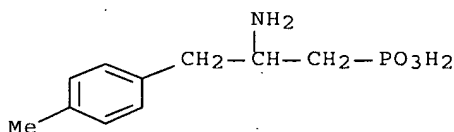
AB   A simple and stereoselective synthesis of primary (E)-allylamines and N-phosphorylated 1-azadienes is reported. N-phosphorylated azadienes were obtained by addn. of ClPPh2 or ClP(OEt)2 to .alpha.,.beta.-unsatd. oximes, while N-(4-methoxyphenyl) azadienes were prepd. by olefination of .beta.-enamino phosphine oxides. Redn. of azadienes and derivs. with hydrides, followed by deprotection of the resulting amines gives primary allylamines and .beta.-amino phosphine oxides, phosphonates, and phosphonic acid derivs.

IT   212388-24-4P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of N-phosphorylated azadienes, primary allylamines, and
       .beta.-amino phosphine oxides and -phosphonates from oximes)

RN   212388-24-4 CAPLUS

CN   Phosphonic acid, [2-amino-3-(4-methylphenyl)propyl]- (9CI)   (CA INDEX
    NAME)

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

sphingosine-1-phosphate (S1P) and by a phosphoryl metabolite of the
immunosuppressive agent FTY720. Both species were high-affinity agonists of
at least four of the five S1P receptors. These agonists produce lymphopenia
in blood and thoracic duct lymph by sequestration of lymphocytes in lymph
nodes, but not spleen. S1P receptor agonists induced emptying of lymphoid
sinuses by retention of lymphocytes on the abluminal side of sinus-lining
endothelium and inhibition of egress into lymph. Inhibition of lymphocyte
recirculation by activation of S1P receptors may result in therapeutically
useful immunosuppression.
IT   402615-93-4
      RL: PAC (Pharmacological activity); BIOL (Biological study)
          (alteration of lymphocyte trafficking by sphingosine-1-phosphate
          receptor agonists)
RN   402615-93-4 CAPLUS
CN   Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]-
      (9CI) (CA INDEX NAME)
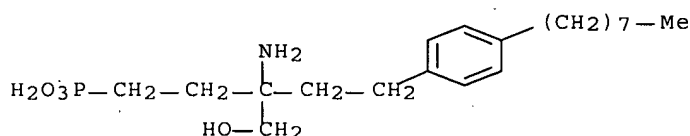
REFERENCE COUNT: 26   THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:171909 CAPLUS Full-text
DOCUMENT NUMBER: 136:216887
TITLE: Preparation of phosphate derivatives as
                            immunosuppressants
INVENTOR(S):   Mandala, Suzanne; Bergstrom, James; Hajdu, Richard;
                            Rosen, Hugh; Parsons, William H.; Card, Deborah J.;
                            Maccoss, Malcolm .
PATENT ASSIGNEE(S):   Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 59 pp.
                            CODEN: PIXXD2
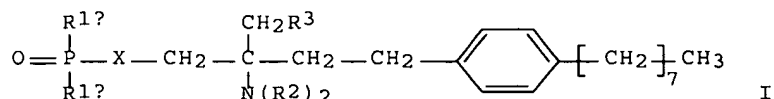DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002018395	A1	20020307	WO 2001-US26789	20010828

      W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
          CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
          GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
          LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT,
          RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
          UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
      RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
          DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
          BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| CA 2421893 | A1 | 20020307 | CA 2001-2421893 | 20010828 |
| AU 2001085331 | A5 | 20020313 | AU 2001-85331 | 20010828 |

O=P—X—CH₂—C—CH₂—CH₂—⟨benzene⟩—[CH₂]₇—CH₃   I

$$O\!=\!\underset{R1?}{\overset{R1?}{P}}\!-\!X\!-\!CH_2\!-\!\underset{N(R2)_2}{\overset{CH_2R^3}{C}}\!-\!CH_2\!-\!CH_2\!-\!\bigcirc\!-\![CH_2]_7\!-\!CH_3 \qquad I$$

AB   Immunoregulatory compds. [I; wherein: X = O, S, NR1, (CH2)1-2, optionally
        substituted with 1-4 halo groups (R1 = H, (C1-C4)alkyl, (C1-C4)haloalkyl); R1a
        = H, OH, (C1-C4)alkyl, (C1-C4)alkyloxy, the alkyl and alkyloxy portions being
        optionally substituted with 1-3 halo groups; R1b = H, OH, (C1-C4)alkyl, (C1-
        C4)haloalkyl; R2 = H, (C1-C4)alkyl, (C1-C4)haloalkyl; and R3 = H, OH, halo,
        (C1-C4)alkyloxy, (C1-C4)haloalkyloxy], as well as the pharmaceutically
        acceptable salts and hydrates thereof, are disclosed. Thus, a multistep prepn.
        of 3-amino-3-hydroxymethyl-5-(4- octylphenyl)pentylphosphonic acid is
        described. The compds. are useful as immunosuppressants, particularly in the
        treatment of bone marrow and organ transplant rejection. Pharmaceutical
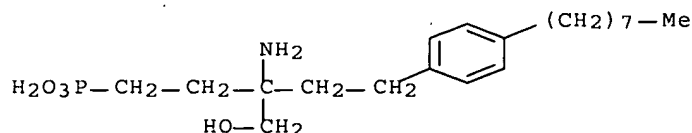   compns. and methods of use are included.
IT   402615-93-4P 402615-95-6P 402615-99-0P
        402616-00-6P 402616-04-0P 402616-06-2P
        402616-10-8P 402616-11-9P 402616-14-2P
        402616-15-3P 402616-18-6P 402616-20-0P
        402616-25-5P
        RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
        (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (Uses)
            (prepn. of phosphate derivs. as immunosuppressants)
RN   402615-93-4 CAPLUS
CN   Phosphonic acid, [3-amino-3-(hydroxymethyl)-5-(4-octylphenyl)pentyl]-
        (9CI) (CA INDEX NAME)

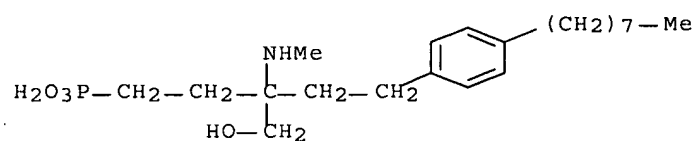$$H_2O_3P\!-\!CH_2\!-\!CH_2\!-\!\underset{\underset{CH_2}{\overset{|}{HO}}}{\overset{NH_2}{C}}\!-\!CH_2\!-\!CH_2\!-\!\bigcirc\!-\!(CH_2)_7\!-\!Me$$

RN   402615-95-6 CAPLUS
CN   Phosphonic acid, [4-amino-4-(hydroxymethyl)-6-(4-octylphenyl)hexyl]- (9CI)

$$\text{H}_2\text{O}_3\text{P}-(\text{CH}_2)_3-\overset{\overset{\displaystyle \text{NH}_2}{|}}{\underset{\underset{\displaystyle \text{HO}-\text{CH}_2}{|}}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{C}_6\text{H}_4-(\text{CH}_2)_7-\text{Me}$$
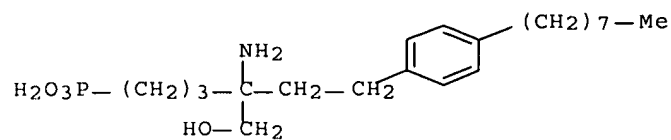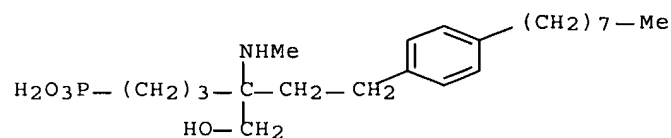
RN   402615-99-0   CAPLUS
CN   Phosphonic acid, [3-(hydroxymethyl)-3-(methylamino)-5-(4-
      octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)
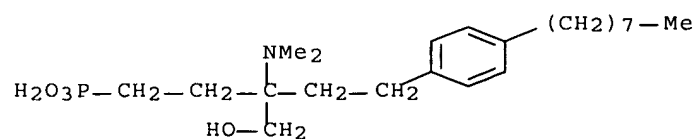
$$\text{H}_2\text{O}_3\text{P}-\text{CH}_2-\text{CH}_2-\overset{\overset{\displaystyle \text{NHMe}}{|}}{\underset{\underset{\displaystyle \text{HO}-\text{CH}_2}{|}}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{C}_6\text{H}_4-(\text{CH}_2)_7-\text{Me}$$

RN   402616-00-6   CAPLUS
CN   Phosphonic acid, [4-(hydroxymethyl)-4-(methylamino)-6-(4-
      octylphenyl)hexyl]- (9CI)   (CA INDEX NAME)

$$\text{H}_2\text{O}_3\text{P}-(\text{CH}_2)_3-\overset{\overset{\displaystyle \text{NHMe}}{|}}{\underset{\underset{\displaystyle \text{HO}-\text{CH}_2}{|}}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{C}_6\text{H}_4-(\text{CH}_2)_7-\text{Me}$$
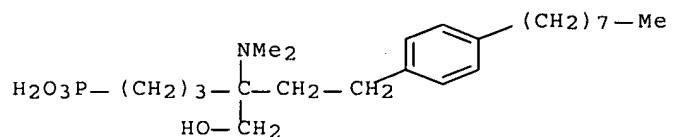
RN   402616-04-0   CAPLUS
CN   Phosphonic acid, [3-(dimethylamino)-3-(hydroxymethyl)-5-(4-
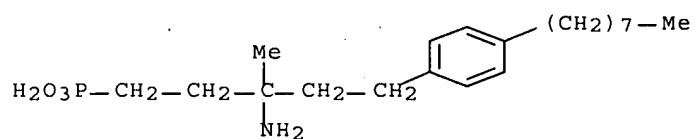   octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)

$$\text{H}_2\text{O}_3\text{P}-\text{CH}_2-\text{CH}_2-\overset{\overset{\displaystyle \text{NMe}_2}{|}}{\underset{\underset{\displaystyle \text{HO}-\text{CH}_2}{|}}{\text{C}}}-\text{CH}_2-\text{CH}_2-\text{C}_6\text{H}_4-(\text{CH}_2)_7-\text{Me}$$

RN   402616-06-2   CAPLUS
CN   Phosphonic acid, [4-(dimethylamino)-4-(hydroxymethyl)-6-(4-
      octylphenyl)hexyl]- (9CI)   (CA INDEX NAME)
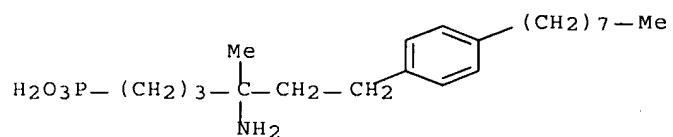
$$H_2O_3P-(CH_2)_3-\overset{\overset{\displaystyle NMe_2}{|}}{\underset{\underset{\displaystyle HO-CH_2}{|}}{C}}-CH_2-CH_2-\text{C}_6H_4-(CH_2)_7-Me$$

RN   402616-10-8   CAPLUS
CN   Phosphonic acid, [3-amino-3-methyl-5-(4-octylphenyl)pentyl]- (9CI)   (CA
      INDEX NAME)

$$H_2O_3P-CH_2-CH_2-\overset{\overset{\displaystyle Me}{|}}{\underset{\underset{\displaystyle NH_2}{|}}{C}}-CH_2-CH_2-\text{C}_6H_4-(CH_2)_7-Me$$

RN   402616-11-9   CAPLUS
CN   Phosphonic acid, [4-amino-4-methyl-6-(4-octylphenyl)hexyl]- (9CI)   (CA
      INDEX NAME)

$$H_2O_3P-(CH_2)_3-\overset{\overset{\displaystyle Me}{|}}{\underset{\underset{\displaystyle NH_2}{|}}{C}}-CH_2-CH_2-\text{C}_6H_4-(CH_2)_7-Me$$
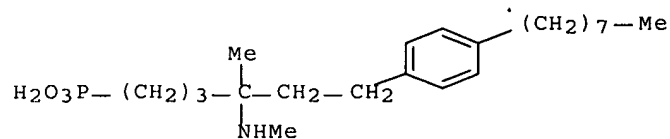
RN   402616-14-2   CAPLUS
CN   Phosphonic acid, [3-methyl-3-(methylamino)-5-(4-octylphenyl)pentyl]- (9CI)
      (CA INDEX NAME)

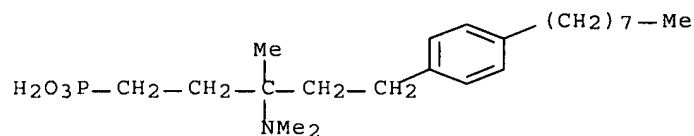$$H_2O_3P-CH_2-CH_2-\overset{\overset{\displaystyle Me}{|}}{\underset{\underset{\displaystyle NHMe}{|}}{C}}-CH_2-CH_2-\text{C}_6H_4-(CH_2)_7-Me$$
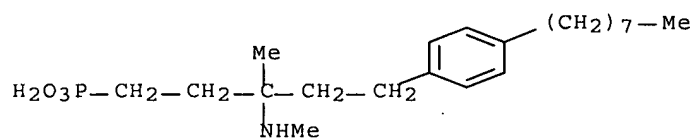
RN   402616-15-3   CAPLUS
CN   Phosphonic acid, [4-methyl-4-(methylamino)-6-(4-octylphenyl)hexyl]- (9CI)
      (CA INDEX NAME)

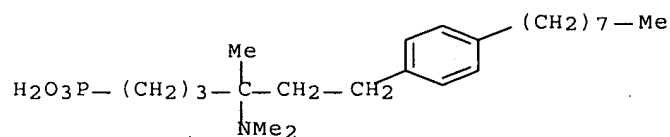$$H_2O_3P-(CH_2)_3-\underset{\underset{NHMe}{|}}{\overset{\overset{Me}{|}}{C}}-CH_2-CH_2-\!\!\!\left\langle \text{phenyl} \right\rangle\!-(CH_2)_7-Me$$

RN   402616-18-6   CAPLUS
CN   Phosphonic acid, [3-(dimethylamino)-3-methyl-5-(4-octylphenyl)pentyl]-
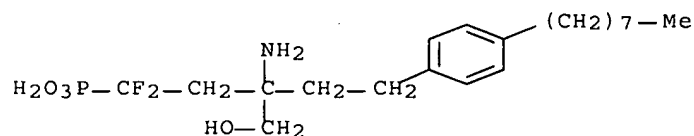   (9CI)   (CA INDEX NAME)

$$H_2O_3P-CH_2-CH_2-\underset{\underset{NMe_2}{|}}{\overset{\overset{Me}{|}}{C}}-CH_2-CH_2-\!\!\!\left\langle \text{phenyl} \right\rangle\!-(CH_2)_7-Me$$

RN   402616-20-0   CAPLUS
CN   Phosphonic acid, [4-(dimethylamino)-4-methyl-6-(4-octylphenyl)hexyl]-
        (9CI)   (CA INDEX NAME)

$$H_2O_3P-(CH_2)_3-\underset{\underset{NMe_2}{|}}{\overset{\overset{Me}{|}}{C}}-CH_2-CH_2-\!\!\!\left\langle \text{phenyl} \right\rangle\!-(CH_2)_7-Me$$

RN   402616-25-5   CAPLUS
CN   Phosphonic acid, [3-amino-1,1-difluoro-3-(hydroxymethyl)-5-(4-
        octylphenyl)pentyl]- (9CI)   (CA INDEX NAME)

$$H_2O_3P-CF_2-CH_2-\underset{\underset{HO-CH_2}{|}}{\overset{\overset{NH_2}{|}}{C}}-CH_2-CH_2-\!\!\!\left\langle \text{phenyl} \right\rangle\!-(CH_2)_7-Me$$

REFERENCE COUNT: 2   THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:455564 CAPLUS Full-text
DOCUMENT NUMBER: 129:216686
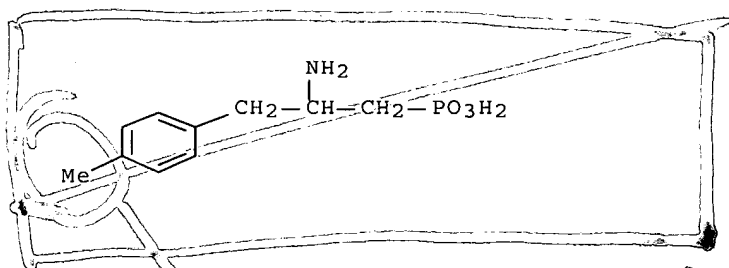TITLE: An efficient synthesis of N-phosphorylated azadienes,

AB   A simple and stereoselective synthesis of primary (E)-allylamines and N-phosphorylated 1-azadienes is reported. N-phosphorylated azadienes were obtained by addn. of ClPPh2 or ClP(OEt)2 to .alpha.,.beta.-unsatd. oximes, while N-(4-methoxyphenyl) azadienes were prepd. by olefination of .beta.-enamino phosphine oxides. Redn. of azadienes and derivs. with hydrides, followed by deprotection of the resulting amines gives primary allylamines and .beta.-amino phosphine oxides, phosphonates, and phosphonic acid derivs.

IT   212388-24-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of N-phosphorylated azadienes, primary allylamines, and
         .beta.-amino phosphine oxides and -phosphonates from oximes)
RN   212388-24-4 CAPLUS
CN   Phosphonic acid, [2-amino-3-(4-methylphenyl)propyl]- (9CI) (CA INDEX NAME)

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.51	581.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.24	-6.24